

Phenol, 4-chloro-2-methoxy-
16766-30-6 | DTXSID0074974

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 238 °C

Global applicability domain: Inside

Local applicability domain index: 6.22e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

Image not found

Phenol, 4-chloro-2-methoxy-

Measured: 241

Predicted: 238

Image not found

2-Ethoxyphenol

Measured: 217

Predicted: 239

Image not found

p-Chlorophenethylic alcohol

Measured: 259

Predicted: 244

Image not found

2-Methoxy-4-methylphenol

Measured: 221

Predicted: 240